Modeling the interconnections between a structural transformation front and a growing crack

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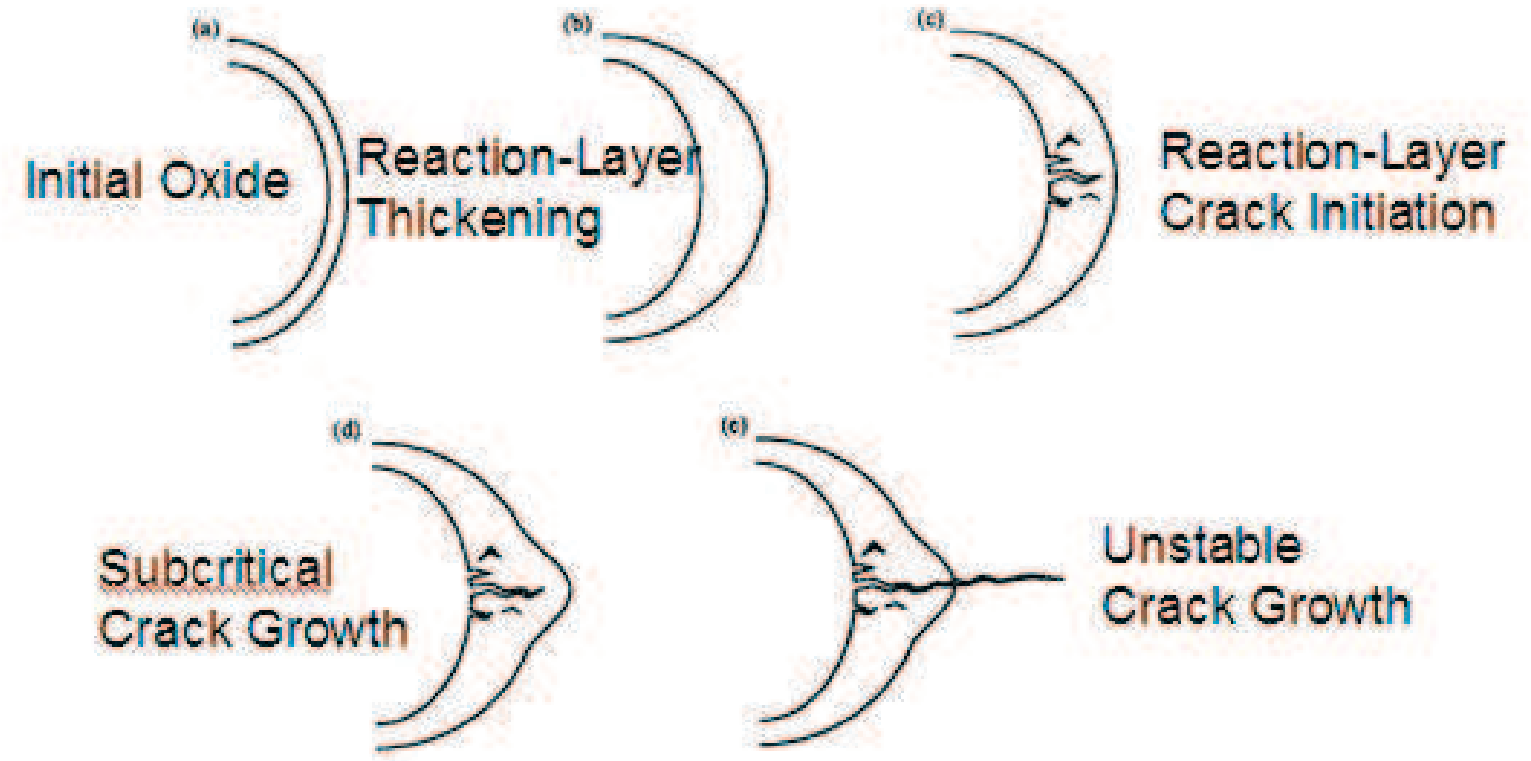
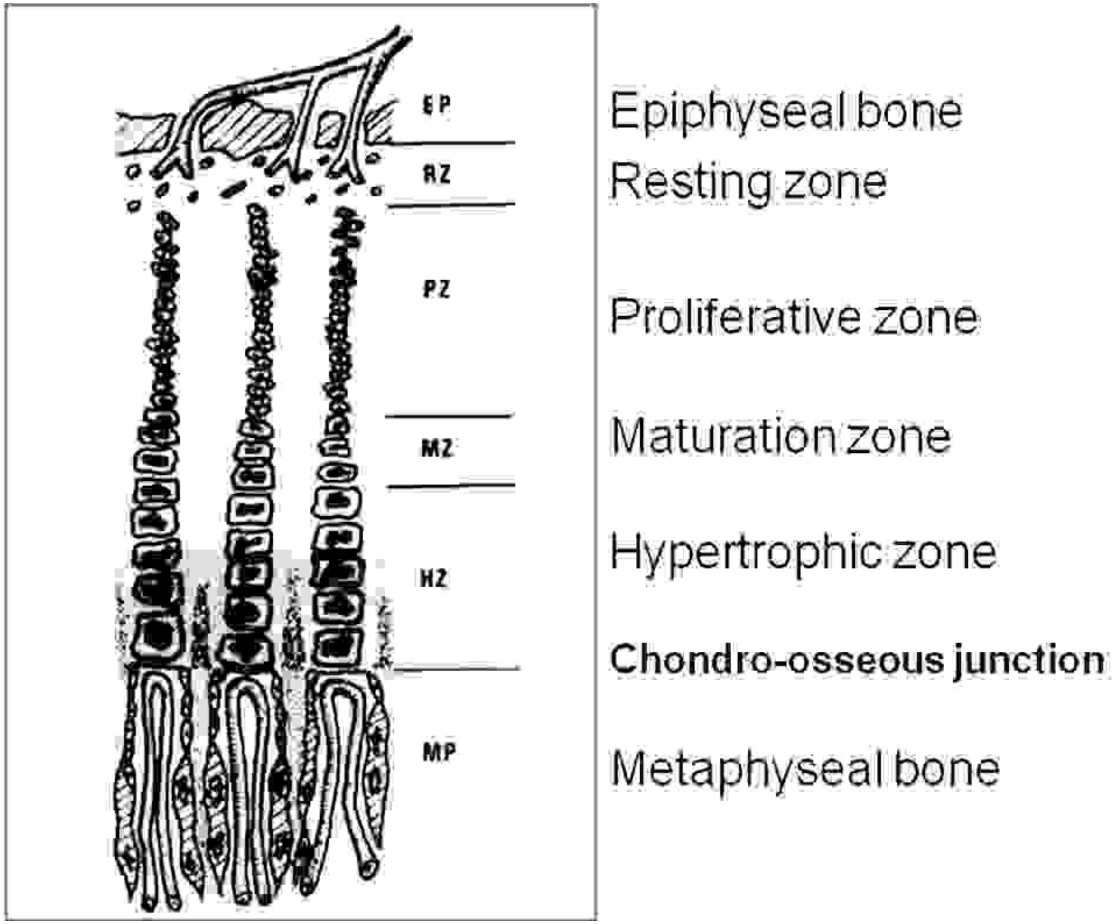
Motivation: MEMS applications

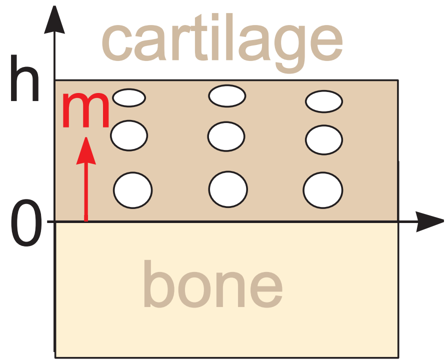
High-cycle fatigue of micron-scale polycrystalline silicon films: the role of the silica (SiO_2)/silicon (Si) interface



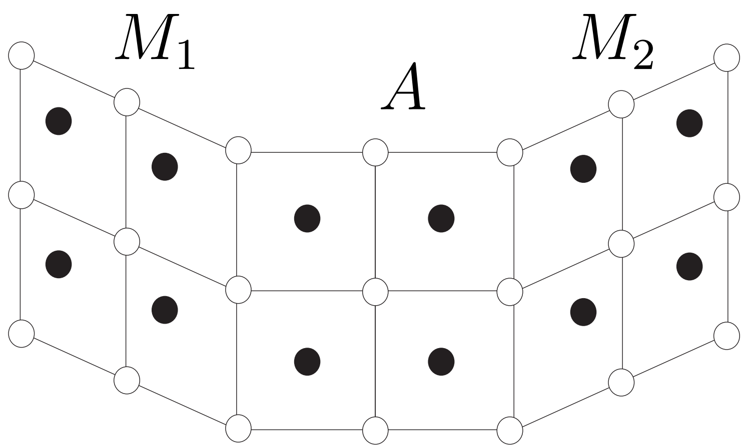
Experiment: Muhlstein *et al* (2001,2002...)

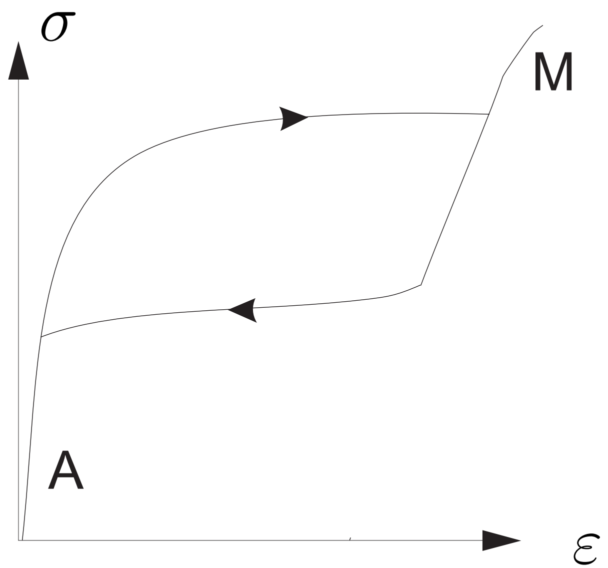
Bone growth and a growth plate





Motivation: martensite transformations, superelasticity, shape memory effects





Austenite A and martensite variants M_1, M_2

$A \leftrightarrows M_1, M_2$ — transformation strains

M_1, M_2 — twining

General motivation: materials with variable structures

Two approaches

- ◇ Variants of plasticity (inelasticity) with internal parameters — do not see interfaces
- ◇ Considering two phase structures and corresponding local stresses — unknown interfaces, nonconvex energy, non-uniqueness, stability

When, what, where and how?

I keep six honest serving-men:

(They taught me all I knew)

Their names are What and Where and When

And How and Why and Who.

Rudyard Kipling. *The Elephant's Child*

- Given a material and a straining path, *why*, *when*, *what* and *where* two-phase structures can appear?
- How a material transforms from one phase state to another?

Construction of transformation ("yield") surfaces. Direct and reverse transformations.
The orientation and the shape of the interfaces. Boundary value problems. Non-uniqueness. Stability.
Heterogeneous deformation due to multiple appearance of new phase domains.
Relationships between local and external strains. Macro-constitutive equations (average strain – average stress).

Our recent publications (selected)

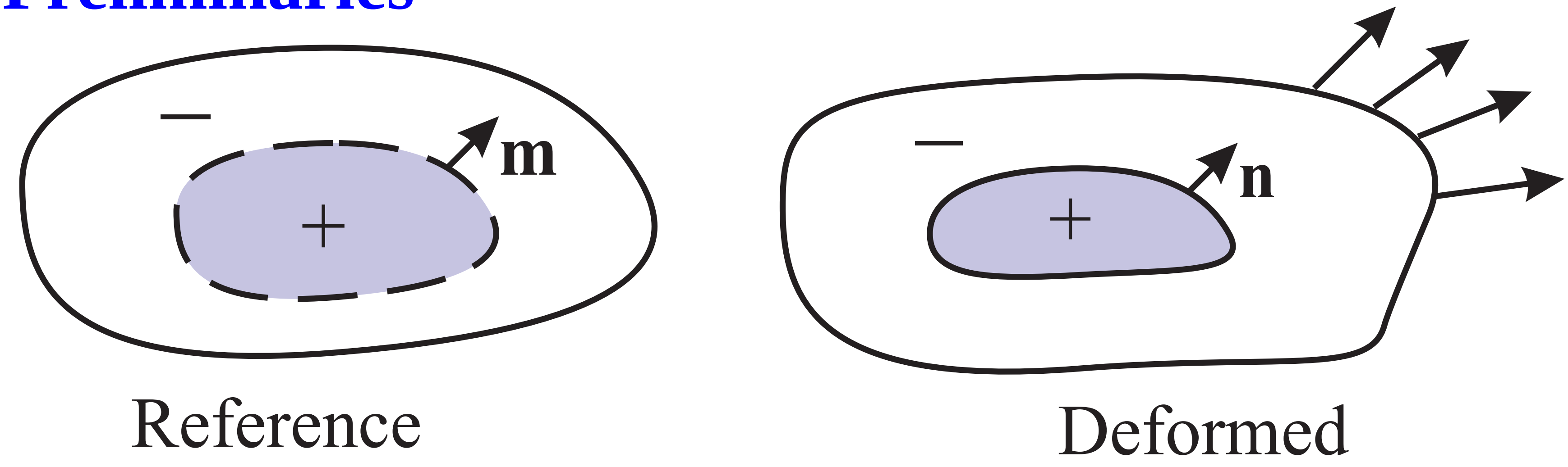
1. A.B.Freidin, E.N.Vilchevskaya. Multiple development of new phase inclusions in elastic solid. *Int. J. Engineering Sciences*, **47** (2009) 240-260.
2. E.N. Vilchevskaya, A.B. Freidin. On phase transformations in a material inhomogeneity, *Mechanics of Solids. (MTT)* **42** (2007)
3. V.A. Eremeyev, A.B. Freidin, L.L. Sharipova. The stability of the equilibrium of two-phase elastic solids. *Journal of Applied Mathematics and Mechanics (P.M.M.)*, **71** (2007) 61-84.
4. A.B. Freidin. On new phase inclusions in elastic solids. *ZAMM*, **87** (2007) 102-116.
5. A.B. Freidin, Y.B. Fu, L.L. Sharipova, E.N. Vilchevskaya Spherically symmetric two-phase deformations and phase transition zones, *IJSS*, **43** (2006) 4484-4508.
6. A.B. Freidin, L.L. Sharipova, On a model of heterogeneous deformation of elastic bodies by the mechanism of multiple appearances of new phase layers, *Meccanica*, **41** (2006) 321-339.
7. Y.B. Fu, A.B. Freidin. Characterization and stability of two-phase piecewise-homogeneous deformations, *Proc. of the Royal. Soc. Lond.* **A 460** (2004) 3065-3094.

Kinetics of interfaces

- What strains can exist on the interface in a given material and interface velocity (A tool: modified phase transition zones)
- Isolated new phase inclusion. Spherically symmetric two-phase deformations. Multiple growth of new phase areas (laminates and quasi-ellipsoidal inclusions).

  Relaxation times. Relations with stability.
- **Interconnections between advancing crack and a moving interface.**
- **Quasi-statical chemical reactions front propagation.**
- Hysteresis phenomena in SMA and the interface kinetics.

Preliminaries



• Phase boundaries — the surfaces of strain discontinuity at continuous displacements

• A thermodynamic condition has to be put on the equilibrium interface (*Knowles& Abeyaratne*, *Grinfeld*, *James*, *Gurtin*, ...)

• Moving interfaces within the framework of configurational forces mechanics (*Eshelby*, *Knowles& Abeyaratne*, *Maugin*, *Gurtin*,...)

• The type of strain localization due to phase transformations depends on a strain state

Equilibrium and moving interfaces

Free energy: $f(\mathbf{F}, \theta)$

$\theta = \text{const} \Longrightarrow f(\mathbf{F}, \theta) \equiv W(\mathbf{F})$ — strain energy function

- Kinematic compatibility condition: $[\![\mathbf{u}]\!] = 0 \Longrightarrow [\![\mathbf{F}]\!] = \mathbf{f} \otimes \mathbf{m}$
- Traction continuity condition: $[\![\mathbf{S}]\!]\mathbf{m} = 0 \quad (\mathbf{S} = \partial f / \partial \mathbf{F})$
- **Thermodynamic equilibrium**: $[\![f]\!] - \mathbf{f} \cdot \mathbf{S}_{\pm}\mathbf{m} = 0$

$$\mathbf{m} \cdot [\![\mathbf{M}]\!]\mathbf{m} = 0 \Longleftrightarrow [\![\mathbf{M}]\!]\mathbf{m} = 0 \tag{1}$$

$\mathbf{M} = f\,\mathbf{I} - \mathbf{F}^T\mathbf{S}$ — Eshelby stress tensor,

$\mu_m = \mathbf{m} \cdot \mathbf{M}\mathbf{m}, \qquad [\![\mu_m]\!] = 0$

Linear thermodynamics approach: $v_m^\Gamma = -k[\![\mu_m]\!], \; k > 0$

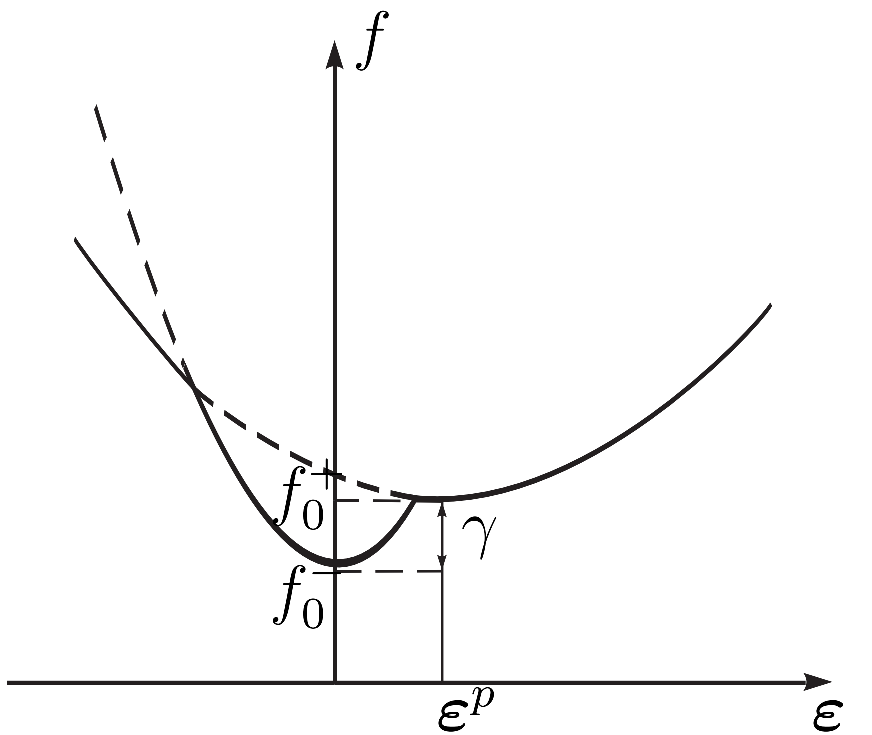
Motivation – non-negativity of dissipation (*Knowles, 1979*)

$$D = -\int_\Gamma v_m^\Gamma \mathbf{m} \cdot [\![\mathbf{M}]\!]\mathbf{m} \mathrm{d}\Gamma > 0$$

Two linear elastic phases

$$f(\boldsymbol{\varepsilon},\theta) = \min_{-,+}\left\{f^{-}(\boldsymbol{\varepsilon},\theta), f^{+}(\boldsymbol{\varepsilon},\theta)\right\} \tag{2}$$

$$f^{\pm}(\boldsymbol{\varepsilon},\theta) = f_0^{\pm}(\theta) + \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p_{\pm}) : \mathbf{C}_{\pm} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p_{\pm})$$



$$\boldsymbol{\sigma}_{\pm}(\boldsymbol{\varepsilon}) = \mathbf{C}_{\pm}:(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p_{\pm}), \quad \text{if} \quad \boldsymbol{\varepsilon}^p_{-} = 0 \Longrightarrow \boldsymbol{\varepsilon}^p_{+} = \boldsymbol{\varepsilon}_p$$

Admissible strains at equilibrium and moving interfaces. Modified phase transition zones

$$\mathbf{x} \notin \Gamma \quad : \qquad \nabla \cdot \boldsymbol{\sigma} = 0, \quad \theta = \text{const}, \tag{3}$$

$$\mathbf{x} \in \Gamma \quad : \qquad [\mathbf{u}] = 0, \quad [\boldsymbol{\sigma}] \cdot \mathbf{n} = 0, \tag{4}$$

$$[\mu_n] \equiv [f] - \boldsymbol{\sigma} : [\boldsymbol{\varepsilon}] = -v_n^{\Gamma}/L \tag{5}$$

The jumps in strain or in stress across the interface can be express through the strain or stress on one side of the interface

$$[\boldsymbol{\varepsilon}] = \mathbf{K}_{-}(\mathbf{n}) : \mathbf{q}_{+}, \quad [\boldsymbol{\sigma}] = \mathbf{S}_{-}(\mathbf{n}) : \mathbf{m}_{+} \tag{6}$$

$$\mathbf{q}_{+} \triangleq -\mathbf{C}_1 : \boldsymbol{\varepsilon}_{+} + \mathbf{C} : \boldsymbol{\varepsilon}^p, \quad \mathbf{m}_{+} \triangleq \mathbf{B}_1 : \boldsymbol{\sigma}_{+} + \boldsymbol{\varepsilon}^p$$

$$\mathbf{K}_{-}(\mathbf{n}) = \{\mathbf{n} \otimes \mathbf{G}_{-}(\mathbf{n}) \otimes \mathbf{n}\}^s, \quad \mathbf{G}_{-}(\mathbf{n}) = (\mathbf{n} \cdot \mathbf{C}_{-} \cdot \mathbf{n})^{-1},$$

$$\mathbf{S}_{-}(\mathbf{n}) = \mathbf{C}_{-} : \mathbf{K}_{-}(\mathbf{n}) : \mathbf{C}_{-} - \mathbf{C}_{-}$$

$$\mathbf{B}_{\pm} = \mathbf{C}_{\pm}^{-1}, \quad \mathbf{C}_1 = \mathbf{C}_{+} - \mathbf{C}_{-}, \quad \mathbf{B}_1 = \mathbf{B}_{+} - \mathbf{B}_{-}$$

Admissible strains at equilibrium and moving interfaces. Modified phase transition zones

$$v_n^\Gamma = -L[\mu_n], \quad [\mu_n] = [f] - \langle \boldsymbol{\sigma} \rangle : [\boldsymbol{\varepsilon}] \tag{7}$$

We express $[\mu_n]$ through stress on one side of the interface and the normal.

$$[\mu_n] = \gamma - \frac{1}{2}\boldsymbol{\sigma}_+ : \mathbf{B}_1 : \boldsymbol{\sigma}_+ - \boldsymbol{\sigma}_+ : \boldsymbol{\varepsilon}^p + \frac{1}{2}\mathbf{m}_+ : \mathbf{S}_-(\mathbf{n}) : \mathbf{m}_+$$

where $\gamma(T) = [f_0]$. If the tensor $\mathbf{C}_1^{-1}$ is nonsingular then

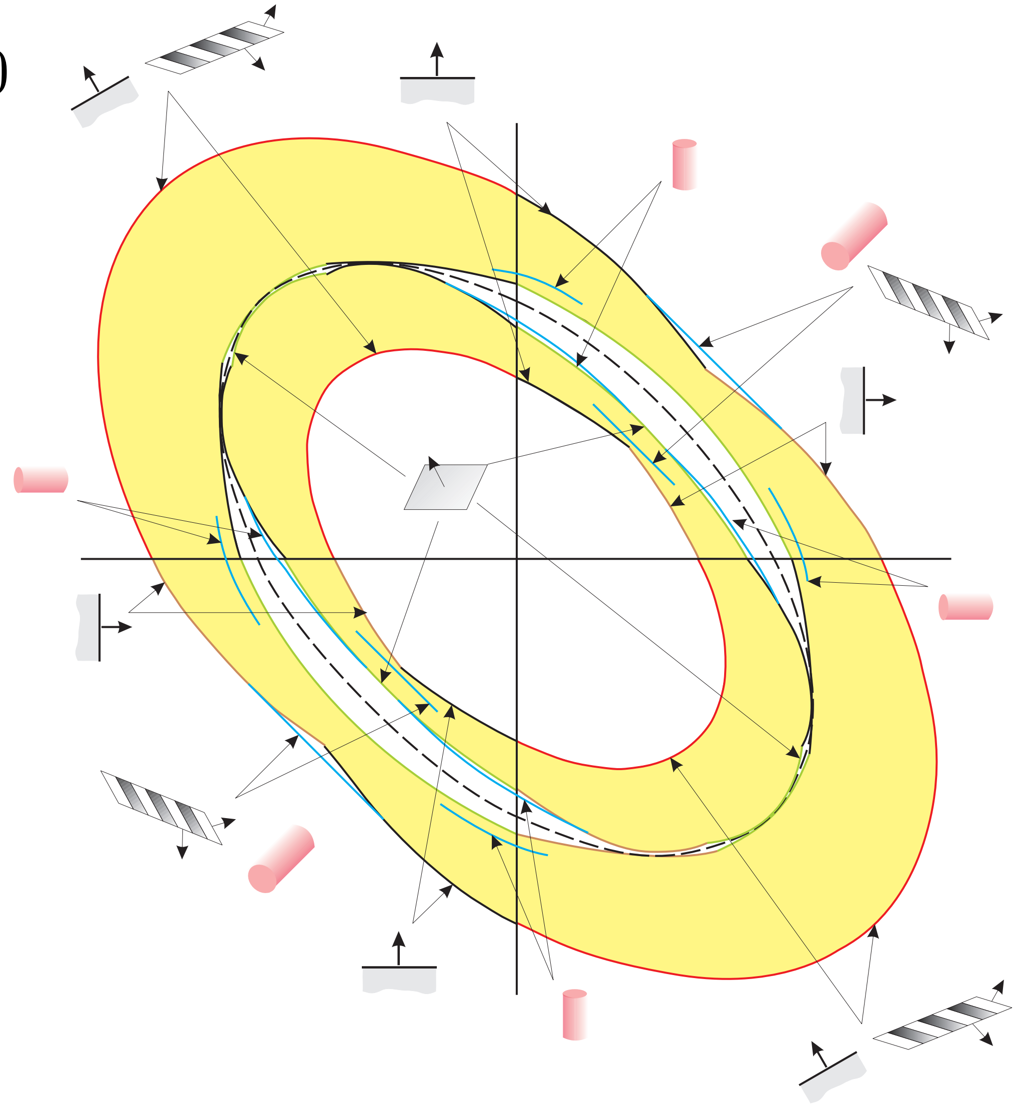
$$[\mu_n] = \gamma_* - \frac{1}{2}\mathbf{m}_+ : \left(\mathbf{B}_1^{-1} - \mathbf{S}_-(\mathbf{n})\right) : \mathbf{m}_+ \tag{8}$$

$$\gamma_* \triangleq \gamma + \frac{1}{2}\boldsymbol{\varepsilon}^p : \mathbf{B}_1^{-1} : \boldsymbol{\varepsilon}^p \tag{9}$$

Strains which can exist on the interface form a phase transition zone (PTZ) in a strain space

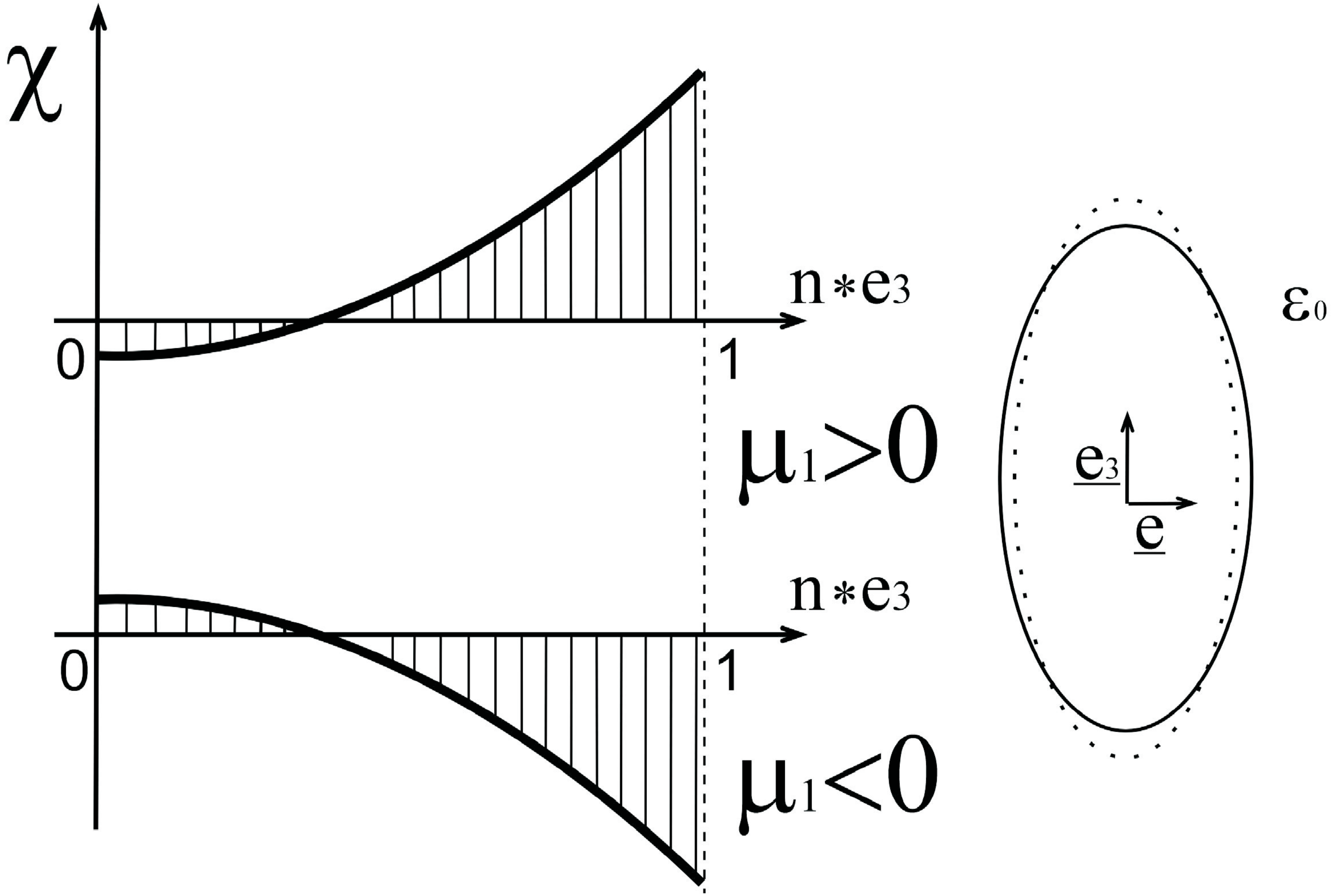
Biaxial external strains

$\mu_1 < 0, K_1 < 0$

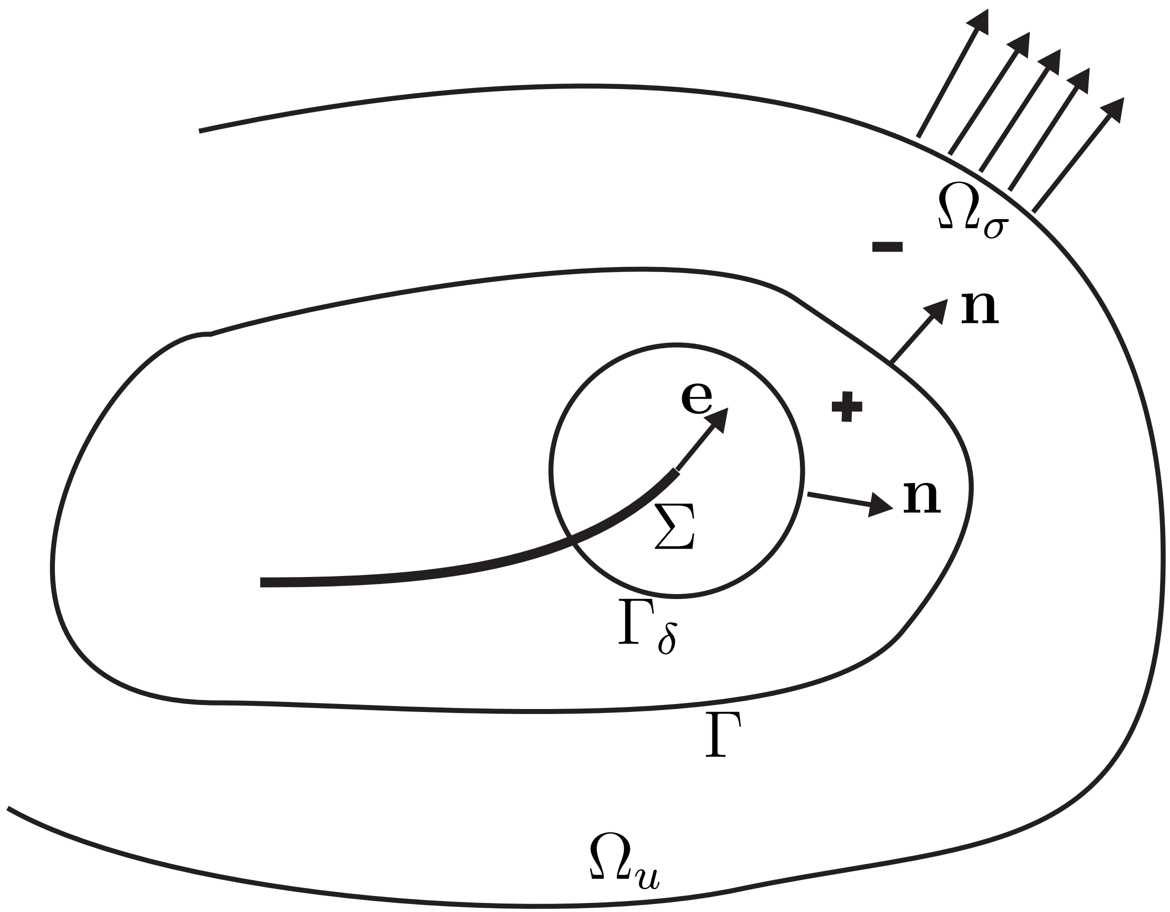


The PTZ — a “passport” of a material that can suffer two-phase deformations, a technique to study how a strain state affects the type of strain localization due to phase transformation.

Configurational forces and kinetics not far from equilibrium



Interconnections between a crack and a phase transformation front.



Entropy production

$$TP[S] = (J - 2\gamma_\Sigma)\dot{l} - \int\limits_\Gamma [\mu_n] v_n^* d\Gamma + D \geq 0$$

$$\mu_n = \mathbf{n}\cdot\mathbf{M}\cdot\mathbf{n}, \quad \mathbf{M} = f\mathbf{E} - \nabla\mathbf{u}\cdot\boldsymbol{\sigma}, \quad M_{ij} = f\delta_{ij} - u_{k,i}\sigma_{kj}$$

$$[\mu_n] = \gamma - \frac{1}{2}\boldsymbol{\sigma}_+ : \mathbf{B}_1 : \boldsymbol{\sigma}_+ - \boldsymbol{\sigma}_+ : \boldsymbol{\varepsilon}^p + \frac{1}{2}\mathbf{m}_+ : \mathbf{S}_-(\mathbf{n}) : \mathbf{m}_+$$

The problem of finding the driving force $[\mu_n]$ acting on the interface is reduced to strain or stress calculations on one side of the interface — determined by the stress intensity factors as well as the Rice integral.

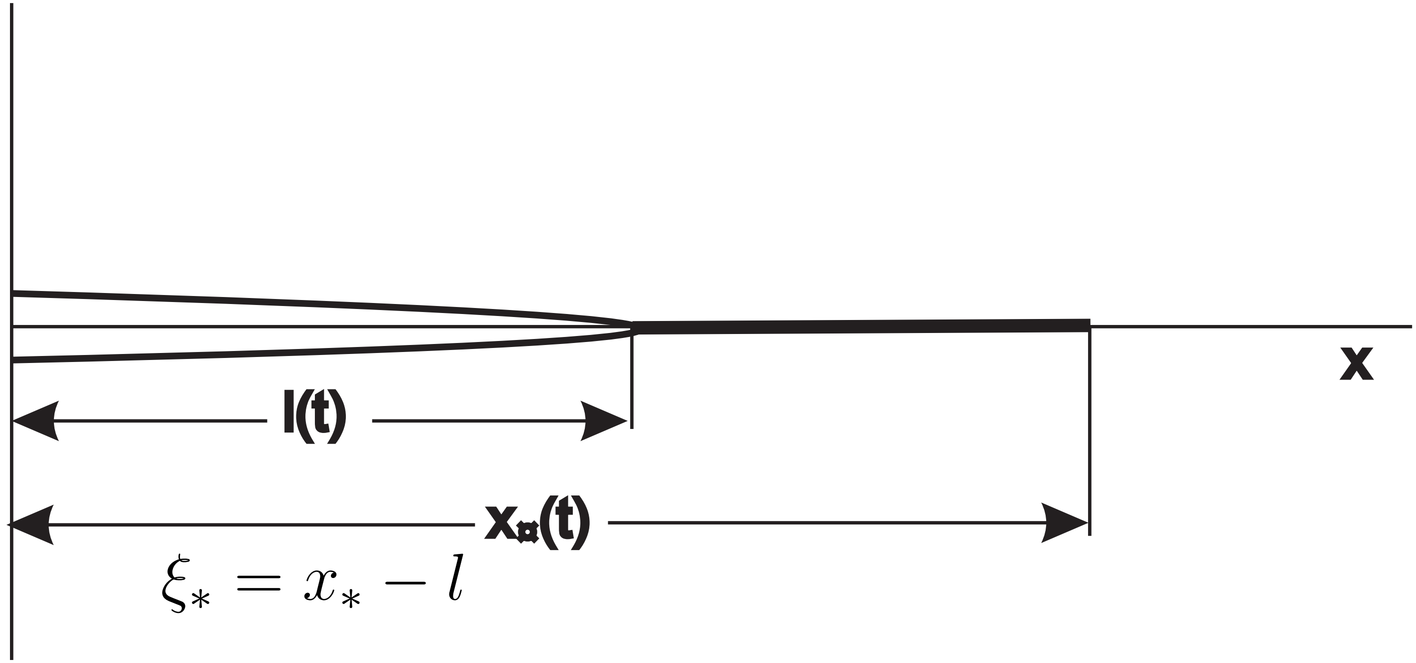
$$\mathbf{C}_- = \mathbf{C}_+ \implies [\mu_n] = \gamma - \boldsymbol{\sigma}_+ : \boldsymbol{\varepsilon}^p + \frac{1}{2}\boldsymbol{\varepsilon}^p : \mathbf{S}(\mathbf{n}) : \boldsymbol{\varepsilon}^p$$

$$\boldsymbol{\varepsilon}^p = (\vartheta^p/2)\mathbf{E}^2$$

$$\boldsymbol{\sigma}_+ : \boldsymbol{\varepsilon}^p = \frac{2K_I\vartheta^p}{\sqrt{2\pi(x_* - l)}}, \qquad \boldsymbol{\varepsilon}^p : \mathbf{S}(\mathbf{n}) : \boldsymbol{\varepsilon}^p = -2a(\vartheta^p)^2, \quad a > 0$$

$$TP[S] = d_*\left(\frac{2K_I\vartheta^p}{\sqrt{2\pi\xi_*}} + a(\vartheta^p)^2 - \gamma\right)v_* - \left(2\gamma_\Sigma - \frac{K_I^2}{E}\right)\dot{l} \geq 0$$

1D-localized phase transformations



$$TP[S] = d_* \left(\mathcal{K}_*(l,\xi_*) - \gamma\right)\dot{\xi}_* - \\ \left(2\gamma_\Sigma - \mathcal{K}_l(l,\xi_*) - d_*(\mathcal{K}_*(l,\xi_*) - \gamma)\right)\dot{l} \geq 0$$

If $\dot{l} > 0$ and $2\gamma_\Sigma - \mathcal{K}_l(l,\xi_*) > d_*(\mathcal{K}_*(l,\xi_*) - \gamma)$ then $\dot{\xi}_* > 0$, the transformation front moves away from the crack tip.

If $\xi_* \to 0$ then $K_I^2/E \to 2\gamma_\Sigma$ (the Griffits crack length).

• Interconnections between the sub-critical crack growth and the transformation front development.

Local fracture criterium

Local fracture takes place if the entropy accumulated due to irreversible processes reaches a critical level (*Chudnovsky, 1973*):

$$\int_{t_s}^{t_f} \sigma\{s\}(x,t')dt' = s_* \tag{10}$$

$\sigma\{s\}(x,t')-$ the entropy production density

t_s- the start time of the dissipative processes at the point x

t_f- the point x is captured by the fracture front.

Entropy fracture criterium

$$T\sigma\{s\}(x,t') =$$

$$(J(t') - 2\gamma_\Sigma)\dot{l}\delta(x - l(t')) + \omega v_*\delta(x_*(t') - x) + R(x,t') \quad (11)$$

$$J(l = x) - 2\gamma_\Sigma + \omega(x_* = x) + \Theta(x,t) = Ts_* \quad (12)$$

$$\Theta = \int_{t_s}^{t_f} R(x,t')dt', \quad R(x,t') = \boldsymbol{\psi} : \dot{\boldsymbol{\varepsilon}}^p \quad (13)$$

ω – entropy production at the transformation front at a moment when the front passes via the point x

$J(l = x)$ is calculated at a moment when a crack reaches the point x.

• The crack growth is determined not only by processes at the fracture front but also by the level of preparatory entropy storage.

Example: subcritical crack growth

• The dissipation R is localized in a crack tip vicinity ΔV with a characteristic size b.

• $\Theta = R\Delta t$ where $\Delta t = b/\dot{l}$ is fracture time of the volume ΔV.

If $R = J/\tau$ where τ is a characteristic time then

$$\Theta = \frac{\zeta}{\dot{l}} J, \quad \zeta = b/\tau \tag{14}$$

$$\dot{l} = \frac{\zeta J}{T s_* + 2\gamma_\Sigma + \omega - J} \tag{15}$$

$$l_* : \quad J = T s_* + 2\gamma_\Sigma + \omega, \qquad cf.: \; J = J_c$$

$$\frac{T s_* + 2\omega}{T s_* + \omega + 2\gamma_\Sigma - J} \zeta J + \omega \dot{\xi}_* \geq 0 \tag{16}$$

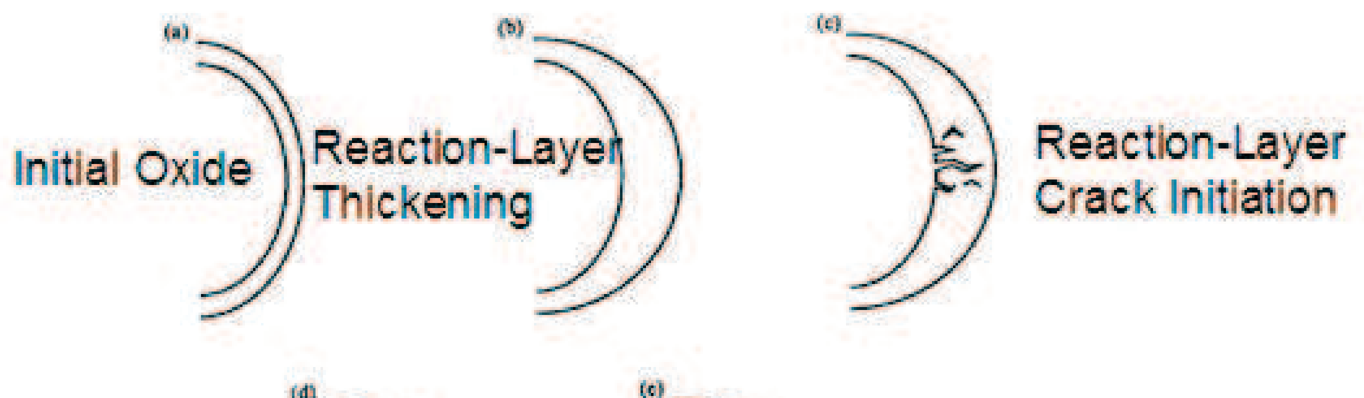
Stress-assist chemical reactions front propagation.

- Chemical reactions of oxidizing type.
- The reaction is localized at the chemical reaction front.
- Reaction is sustained by the diffusion of an oxidizing gas constituent through the solid oxide.

$$\nu_- A_- + \nu_* A_* \to \nu_+ A_+ \tag{17}$$

$A_\pm$ – chemical formulae of solid constituents, A_* – gas
ν_-, ν_*, ν_+ – stoichiometric coefficients.

Example: $\mathrm{Si} + \mathrm{O}_2 \to \mathrm{SiO}_2 \quad (\nu_- = \nu_* = \nu_+ = 1)$



Chemistry background. Chemical affinity

$TP_{\text{chem}}[S] = wA,\quad w-$ chemical reactions rate

$$A = \sum \nu_k M_k \mu_k \tag{18}$$

M_k – molar mass

μ_k – chemical potential per unit mass of the k-th component

ν_k – with the sign "+" if the k-th component is produced; with the sign "−" in the other case.

Kinetics: chemical reactions rate

$$w = w\,(A), \qquad w(0) = 0$$

Chemical reaction front propagation

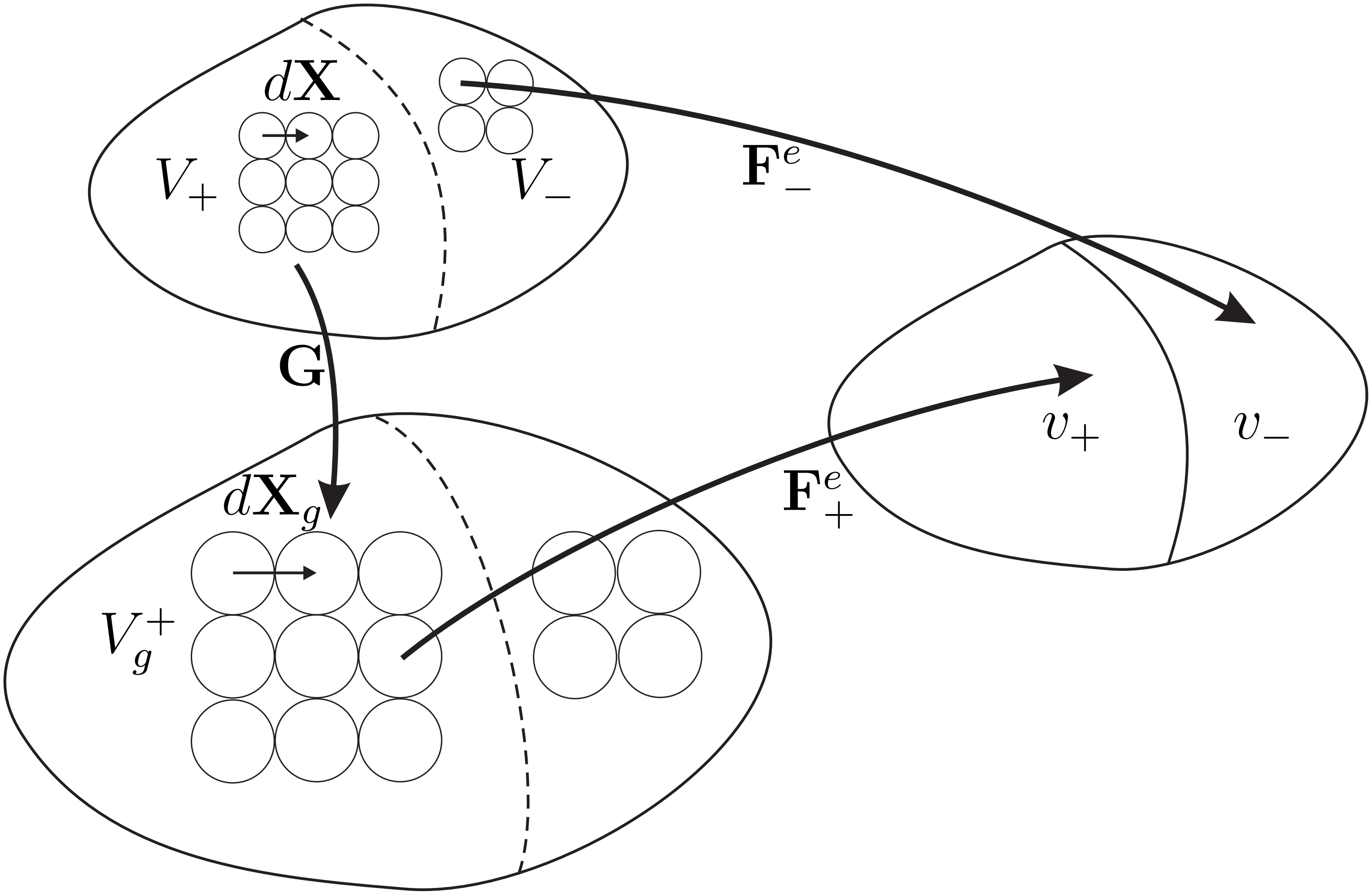
$$TP_{\text{chem}}[S] = v^{\Gamma} A, \qquad v^{\Gamma} = \Phi\,(A)$$

Linear thermodynamic approach: $v^{\Gamma} = -\varkappa A,\quad \varkappa > 0$

Kinematics

$$\nu_- A_- + \nu_* A_* \rightarrow \nu_+ A_+$$

$$d\mathbf{x}_- = \mathbf{F}^e_- \cdot d\mathbf{X}_-, \quad d\mathbf{x}_+ = \mathbf{F}^e_+ \cdot d\mathbf{X}^+_g \tag{19}$$



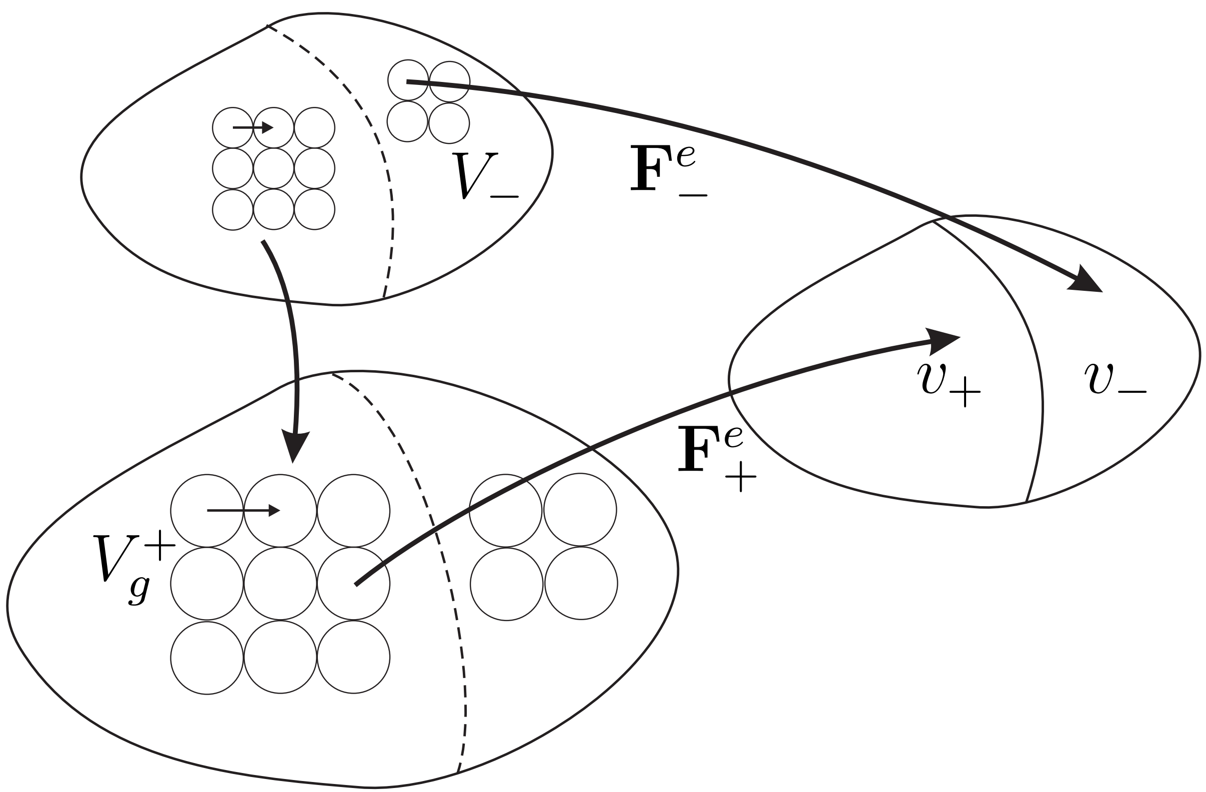
Configurations resulting from the chemical reactions and deformation

- Opened system
- Three configurations: V_0, V_g, v_t.

Elastic strains

$$d\mathbf{x}_- = \mathbf{F}^e_- \cdot d\mathbf{X}_-, \quad d\mathbf{x}_+ = \mathbf{F}^e_+ \cdot d\mathbf{X}_g^+ \tag{20}$$

$$\det \mathbf{F}^e_- = \frac{dv_-}{dV_-} = \frac{\rho_0}{\rho^t_-}, \quad \det \mathbf{F}^e_+ = \frac{dv_+}{dV_g^+} = \frac{\rho_g}{\rho^t_+} \tag{21}$$



Chemical transformations tensor

$$d\mathbf{X}_g = \mathbf{G}\cdot d\mathbf{X} \tag{22}$$

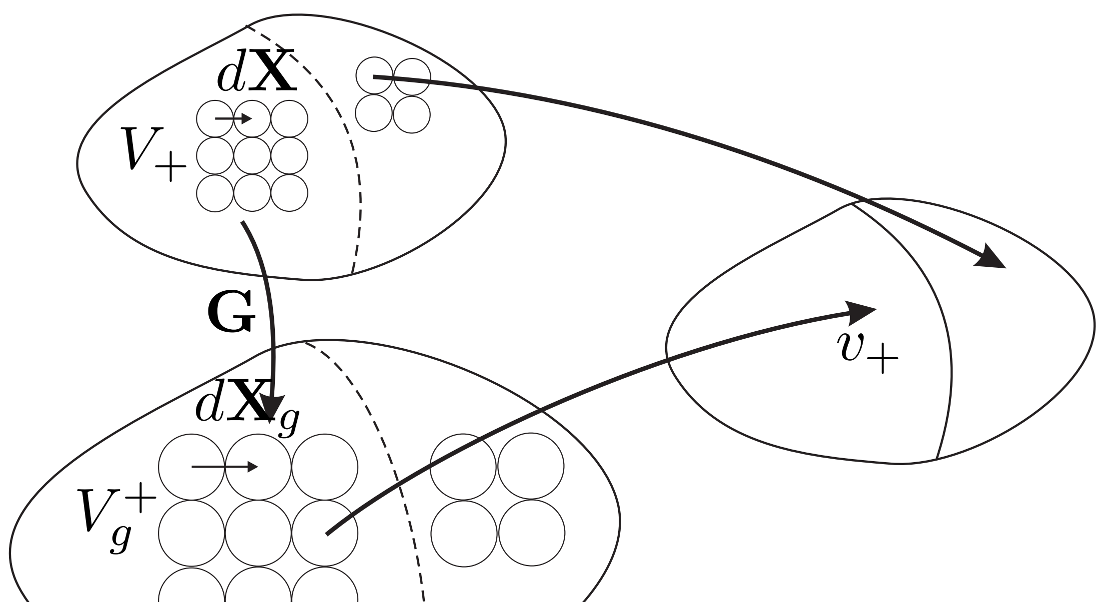
M_- and M_+ – molar masses of constituents A_- and A_+

$dV_0 = \nu_- M_-/\rho_0 \longrightarrow dV_g = \nu_+ M_+/\rho_g$

$$\det\mathbf{G} = \frac{dV_g}{dV_0} = \frac{\nu_+ M_+ \rho_0}{\nu_- M_- \rho_g} \equiv g^3, \qquad \det\mathbf{G} \neq \rho_0/\rho_g \tag{23}$$

$$\mathbf{G} = g\mathbf{E}, \quad g = \left(\frac{\nu_+ M_+}{\nu_- M_-}\frac{\rho_0}{\rho_g^+}\right)^{1/3} \tag{24}$$

$$d\mathbf{x}_+ = \mathbf{F}_+\cdot d\mathbf{X}_+, \quad \mathbf{F}_+ = \mathbf{F}_+^e\cdot\mathbf{G} = g\mathbf{F}_+^e \tag{25}$$



Stresses. Constitutive equations.

A solid skeleton approach

$$f_- = f_-(\mathbf{F}^e_-, T), \quad f_+ = f_+(\mathbf{F}^e_+, T), \quad f_* = f_-(\rho_*, T)$$

$$\mathbf{S}_- = \rho_0 \frac{\partial f_-}{\partial \mathbf{F}^e_-}, \quad \mathbf{S}^g_+ = \rho_g \frac{\partial f_+}{\partial \mathbf{F}^e_+}, \quad p_* = \rho_*^2 \frac{\partial f_*}{\partial \rho_*} \tag{26}$$

Energy release due to the chemical reaction front propagation

$$D_{solid} = -\frac{\rho_0}{\nu_- M_-} \int\limits_\Gamma \mathbf{N} \cdot \mathbf{A}_{solid} \cdot \mathbf{v}^\Gamma \, d\Gamma$$

$$\mathbf{A}_{solid} = \nu_+ M_+ \widetilde{\mathbf{M}}_+ - \nu_- M_- \widetilde{\mathbf{M}}_- \tag{27}$$

where

$$\widetilde{\mathbf{M}}_+ = f_+ \mathbf{E} - \frac{1}{\rho_g} (\mathbf{S}^g_+)^T \cdot \mathbf{F}^e_+, \quad \widetilde{\mathbf{M}}_- = f_- \mathbf{E} - \frac{1}{\rho_0} \mathbf{S}^T_- \cdot \mathbf{F}^e_-$$

Chemical affinity tensor

$$\text{Gas constituent } A_* : \qquad \dot{\rho}_* = \widehat{\rho}_* - \overset{g}{\nabla} \cdot (\rho_* \mathbf{v}_*)$$

$$\widehat{\rho}_* \mathbf{v}_g^\Gamma \cdot \mathbf{N}_g \, d\Gamma = \frac{\nu_* M_*}{\nu_+ M_+} \rho_g \mathbf{v}_g^\Gamma \cdot \mathbf{N}_g \, d\Gamma$$

$$TP_{\text{front}}[S] = -\frac{\rho_0}{\nu_- M_-} \int_\Gamma \mathbf{N} \cdot \mathbf{A} \cdot \mathbf{v}^\Gamma \, d\Gamma$$

$$\mathbf{A} = \nu_+ M_+ \widetilde{\mathbf{M}}_+ - \nu_- M_- \widetilde{\mathbf{M}}_- - \nu_* M_* \widetilde{\mathbf{M}}_* \tag{28}$$

$$\widetilde{\mathbf{M}}_+ = f_+ \mathbf{E} - \frac{1}{\rho_0} (\mathbf{S}_+^g)^T \cdot \mathbf{F}_+^e$$

$$\widetilde{\mathbf{M}}_- = f_- \mathbf{E} - \frac{1}{\rho_0} \mathbf{S}_-^T \cdot \mathbf{F}_-^e$$

$$\widetilde{\mathbf{M}}_* = \mu_* \mathbf{E}$$

$$A_{`classic'} = \sum \nu_k M_k \mu_k$$

Kinetics

$$\mathbf{N}\cdot\mathbf{A} = A_N\mathbf{N}, \qquad A_N = \mathbf{N}\cdot\mathbf{A}\cdot\mathbf{N}$$

$$TP_{\mathrm{front}}[S] = -\frac{\rho_0}{\nu_- M_-}\int\limits_{\Gamma} A_N v_N^{\Gamma}\, d\Gamma$$

$$v_N^{\Gamma} = \Phi\,(A_N), \qquad v_N^{\Gamma} = -\kappa A_N, \quad \kappa > 0$$

1D-model

$$f_{\pm}(\varepsilon_{\pm}) = f_0^{\pm} + \frac{1}{2}C_{\pm}\varepsilon_{\pm}^2\sigma_{\pm} = C_{\pm}\varepsilon_{\pm}$$

$$A = \gamma_* + \nu_- M_- G\frac{\sigma^2}{2\rho_0 C_-} - \nu_* M_* \mu_*$$

$$\gamma_* = \frac{\nu_+ M_+}{\rho_g}f_0^+ - \frac{\nu_- M_-}{\rho_0}f_0^-, \quad G = 1 - g\frac{C_-}{C_+}, \quad g = \frac{\nu_+ M_+}{\nu_- M_-}\frac{\rho_0}{\rho_g}$$

Conclusions

• Modified PTZ for stationary moving interfaces. Kinetics not far from equilibrium. Stability. Variety of behaviors in dependence of material parameters.

• Interconnections between a growing crack and advancing phase transformation front — basing on the Eshelby stress concept.

◇ Configuration force acting on the interface in terms of the stress intensity factors, as well as the Rice integral.

◇ Inequalities are derived which must be satisfied in the case of the sub-critical crack growth interconnected with an advancing transformation front.

◇ Subcritical crack growth — entropy criterion of the local fracture is tried.

Conclusions

• Stress-assist chemical reactions front propagation is considered.

◇ The expression of chemical affinity tensor is derived.

◇ Introducing the intermediate reference configuration allowed us to express the chemical potentials in terms of stresses related by the constitutive equations of solid constituents of the reaction.

◇ 1D-model is examined.

◇ Further progress is expected on the way of taking into account cross effects related with interconnections between the deformable solid skeleton and diffusion of a gas constituent.

Acknowledgements

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